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QUARTZ ANALYSIS X-RAY DIFFRACTION WITH COMPUTER CONTROL - COMPUTER PROGRAMS AND EXPLANATIONS

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G. Knight*

ABSTRACT

This report provides the final version of the computer programs developed at the Elliot Lake Laboratory for the x-ray diffraction analysis of quartz and other analytes in mine airborne dust after collection on filters. Detailed explanations have been added to the programs to assist in their further development or rewriting if the computer facilities are updated.

KEYWORDS: respirable dust; dust sampling; quartz analysis; x-ray diffraction; computer controlled analysis

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ANALYSE DU QUARTZ PAR DIFFRACTION DES RAYONS X À L'AIDE DE LA GESTION PAR ORDINATEUR PROGRAMMES INFORMATIQUES ET EXPLICATIONS

G. Knight*

RÉSUMÉ

Ce rapport constitue la version finale des programmes informatiques conçus au Laboratoire d'Elliot Lake pour l'analyse par diffraction des rayons X du quartz et d'autres matières à analyser décelées dans la poussière de mine en suspension dans l'air, après captation dans les filtres. On a ajouté aux programmes des explications détaillées pour aider à leur perfectionnement ou à leur réécriture, advenant le remplacement de l'équipement informatique.

MOTS CLÉS : poussières inhalables; prélèvement de poussières; analyse du quartz; diffraction des rayons X; analyse gérée par ordinateur

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INTRODUCTION

A major health hazard in mines is airborne dust. In many hardrock mines the most hazardous component is silica dust. This can be present in four crystalline and some amorphous varieties. The most common form is crystalline quartz. In the early 1970's the Elliot Lake Laboratory developed a sampling and analytical method for the assessment of quartz and other components of the airborne dust in mines (1). In the early 1970's computer control was added to the analysis system (2). The computer program GKXSR?.FT was developed from a gamma ray spectrometry analysis program (3).

The major advantages of the fully developed system were:

1. Automatic control of number of quartz diffraction lines analysed - required for minimizing the counting time when interference is a frequent problem.
2. Automatic selection of counting time dependent on the amount of quartz on the sample.
3. Minimizing the technical skill and time required in interpreting the results and in references to the supervisor.

The objectives of the computer control system were given by G. Knight (2). The objectives of this report is to describe and document the software used now that G. Knight has been transferred from the Elliot Lake Laboratory and others may have to modify and understand the programs used.

OUTLINE DESCRIPTION OF SOFTWARE

The PDP8 computer has only limited memory size for programs and for running. This necessitated splitting the running program in three parts and severely limited the length of symbols, comments and descriptions that could be used thus rendering the programs, input and output difficult to understand.

The program parts are:

1. Main program GKXMN?.FT
2. Input-output subroutine GKXIO?.FT
3. Diffraction line analysis subroutine GKXSR?.FT
4. Data file input data GKXINO.DA
5. Data file performance check data GKXINI.DA.
6. Auxiliary program for creating the two data files and editing the input data file.—GKXPDO.FT

The ? in the title is replaced by a numeral identifying the particular version. The version numbers reached 9 on some of the revisions and in the last major revision they were all set back to 0. The first and third programs have since each received a minor revision and are on version 1 (1987).

The first three parts are compiled into machine language as GKXMN1.RL; GKXIO0.RL; GKXSR1.RL and loaded together with some library units using:

R. LOADER
<GKXMN1.RL, GKXIO0.RL, GKXSR1.RL/I/O/H/G
where I,O, and H are the required components from the library for handling DATA files on tape and G is the go or run command.

The two data files and the machine language programs are stored on tape, together with the PDP8 system programs. A number of back-up tapes have been prepared.

COMPUTER LANGUAGES DESCRIPTION

The language used is FORTRAN II as supplied by Digital for the OS8 operating system on the PDP8 computer. This language uses a two-stage compiler and the intermediate symbolic machine language, SABR, can be intermixed with Fortran. SABR lines are identified by an S in the first column. Advantage has been taken of this feature for various program features which are not available in simple Fortran.

The main uses of SABR are:

1. Instructions for digital input and output.
2. Clock (timing) controls.
3. Reading real time commands from front panel switch register on computer. This includes many of the options: high accuracy, wide peaks, diagnostic output.
4. Use of subroutines within Fortran subroutines (where it is not supported by Fortran II) and programs. This was much simpler than the use of the alternative Fortran GO TO statement.
5. Various routines such as BCD to binary were easier and were used sometimes.

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The author wishes to thank the Elliot Lake Laboratory staff, particularly W. Ropchan, for transferring the file from the PDP8 computer to the VAX computer in Bells Corners ready for word processing to produce this report. The X-ray laboratory staff and temporary students have had some influence on the development of these programs over the many years and their assistance is gratefully acknowledged.

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2. Knight, G. Rapid XRD analysis of quartz in airborne dust samples using computer control, Mining Research Laboratories report MRL 88-2 (J) Revision of MRP/MRL 80-101 (OP,J) (1988).
3. Kemper, A., and G.A. Van Kempen A simple computer program for high resolution gamma ray spectroscopy; J. Radio. Chem. 6 (Dec) 461-475 (1970).

MAIN PROGRAM GKXMN1.

```
C     NAME GKXRMN.FT COMPUTER CONTROL OF XRAY DIFFRACTION
C       added comments are in lower case and refer
C       to the following section or line or follow
C       /UPPER CASE comments ref -ring to existing SABR line
C     FORTRAN AND SABR LANGUAGES
      COMMON A,ANG,NS,C,UK,KU,I,B,Q,LQ,QM,QS,QH,SD,NR,LS
     C,B1,M,M1,MS,L1,L2,LC,BL,BR,HT,AR
      DIMENSION A(8),ANG(20),NS(7),C(29),Q(4),LQ(20),QM(20)
     C,QS(12),QH(12),SD(4,34),NR(12),LS(12),H(94)
C       OPDEF is operation definition; SKPDF skip operation definition
C       DR refers to digital input/output; I is input; Z is zero output
C       for each bit where input bit is one; O is output one for each
C       bit when appropriate bit is one; xxx2 is code call for the
C       third 12 bit output: CLxx are clock controls- read manual;
C       ADxx is analogue to digital input controls- read manual.
S     OPDEF DRI2 6524;OPDEF DRZ2 6525;OPDEF DRO2 6526
S     OPDEF CLZE 6130;OPDEF CLDE 6132;OPDEF CLSA 6135;SKPDF CLSK 6131
S     OPDEF ADCL 6530;OPDEF ADLM 6531;OPDEF ADST 6532;OPDEF ADRB 6533
S     OPDEF ADLE 6536;SKPDF ADSK 6534
C       call subroutine for input data
101   CALL GKXIOP(1)
      KF=I
C       address for restart of program
S     D1,    CLA CLL
C       sample number loop--Standard is number zero -samples 1 to M1
121   DO 100 M=0,M1
C       set output arrays to zero
      DO 105 J=1,12
      NR(J)=0
      QH(J)=0
```

```
105   QS(J)=0
C       call for next sample and interpret sample number from
C       automatic sample changer(ASC) potentiometer
S     JMS NXTSA
      X=MS
      MS=X*A(5)-A(6)
C       selects routine appropriate to standard or sample
      IF(M) 104,103,104
C     ANALYSIS OF STANDARD reference sample always placed in first
C       position on ASC and treated as sample number zero
C       DO loop is for four quartz diffraction lines used
103   DO 132 L2=1,4
C counting time,in clock pulses, for three lines
      KU=10
      IF(L2-2)1031,1032,1031
C ditto for strongest line to avoid counts
C       above 1 000 000 when on high accuracy option
1032  KU=9
1031  UK=ANG(L2)
C       call subroutine for counting and calculation see later
S     JMS CNTCAL
C       check front panel switch register for restart request
S     CLA CLL;OSR;AND (2400;SZA;JMP D1;CLA CLL  /RESTART
C call subroutine for output of standard
      CALL GKXIOP(3)
      H(L2)=HT
132   A(L2)=AR
      GO TO 100
C     LIGHT SAMPLE CORRECTION factor(LSCF) when sample weight below
C       0.4 mg the analysis is non linear
104   FW=1.
C       read front panel switch register for  LSCF omission command
```

```
C       sets LC=1(normal) for 5um pore size silver membrane filters
C       or 0 for 1.2um or finer silver and all plastic filters
S     CLA CLL;DCA \LC;OSR;AND (0040;SZA;JMP D2;IAC;DCA \LC  /LSCF CONT
      W1=SD(4,M)
      IF(W1-.4)1041,1041,1042
1041  X=1.4-W1*(1.4-W1)
      IF(KF-1)1044,1043,1042
1043  X=SQRT(X)
1044  FW=X
C       end of LSCF calculation; final address for skip command in
C       previous S line
S     D2,    CLA CLL
C    CONTROL FOR QTZ &CRYST &OTHER LINES Analysis is split into sets of
C       4 lines; 1st set is quartz; 2nd crystobalite and 3rd tridymite
1042  DO 125 J=1,4
125   Q(J)=0
      SD(3,M)=-1000.
C       this input from switch register sets L5 to 100,200,or 300 for
C       control of stop on reaching match between 2 lines or running
C       all 4; as well as other functions. Sets L=L8=J2=0
S     CLA CLL;OSR;AND (0300;DCA \L5;DCA \L;DCA \L8;DCA \J2  /DIAG
C       L,L? are variables defining diffraction line and line controls
401   L8=L8+L
C       L1 is last line for analysis -checks for sample finished
      IF(L8-L1)402,106,106
C     DIFF LINES PROCESSED IN BATCHES,J2,OF 4,QTZ CRYST ETC
402   J2=J2+1
403   DO 404 L=1,4
      L9=L+L8
      L2=LS(L9)
      L7=L2-J2*4
C       check for sample finished
```

```
      IF(L9-L1)405,405,404
C       check for line in current set of four
405   IF(L7)406,406,420
C       check if match found and skip rest of lines in set
406   IF(L5)404,407,407
407   CONTINUE
C       jump to subroutine for sample count and calculation
S     JMS SAMCAL
C     SILVER PEAK FOR ABSORBTION CORRECTION
      IF(L2-20)441,442,441
442   SD(3,M)=W
C     PLOT ON SECOND RUN IF NO AGREEMENT ON 1ST this can be a useful
C        diagnostic procedure for interference or machine problem
C        (L5=100) set in switch register prevents time-consuming
C        output on sets of samples with frequent problems
441   IF(L5-100)404,404,409
C       prevents garbage output on X-ray fault
409   IF(I-1)408,408,404
C       outputs line data and plot of angle versus count
408   CALL GKXIOP(4)
404   CONTINUE
      L=5
C     NEXT SAMPLE IF X RAY FAULT set QH=-1003 as coded error indication
C     as required for preventing inclusion in averaging process
420   X=QH(1)+QH(2)+2006.
      IF(X)106,106,428
C     DIAGNOSTICS CONTROL
428   L=L-1
      IF(L5)421,422,423
425   IF(L)401,401,426
426   CONTINUE
C       diagnosis output can be called from front panel for any line or
```

```
C       group of lines- has been useful in detecting system or program
C       problems- not used for a number of years
S     CLA CLL;OSR;AND (0010;SZA;JMS DIAG
421   L5=0
      GO TO 401
C       control for/and repeat analysis of set of quartz or
C       crystobalite lines if no match found
422   IF(J2-2)424,425,401
423   IF(L5-200)401,401,421
424   L5=300
      CALL GKXIOP(6)
S     JMS DIAG
      GO TO 403
C       normal sample analysis output procedure
106   CALL GKXIOP(6)
C       check  switch register for finish-analysis-after-
C       -current-sample request
S     CLA CLL;OSR;AND (1000;SZA;JMP TA2;CLA CLL  /FIN & NEW SAMP
100   CONTINUE
C     FINAL TABLE outputs summary of results for all samples
      M=M1
S     TA2,   CLA CLL
      CALL GKXIOP(7)
C       goes to start ready to receive next batch of samples
      GO TO 101
C     END OF PROGRAM SUBROUTINES FOLLOW
S     NXTSA, 0000 /NeXT SAMPLE SubRoutine puts out pulse to
C       initiate automatic sample changer and await clearing of
C       DSCBS (D1 H808#6 Table 6 interface manual) signal from
C       sample changer(DSCBS 0 is busy 1 clear- check PW1394 manual)
C       there are six operations carried out:-
C       1, set two bits (octal 0140 ) in board 2 to zero
```

```
C       2, set two bits (octal 0420 ) in board 2 to one
S     CLA CLL;TAD MB;TAD MR;DRZ2;CLA CLL;TAD MG;DRO2;CLA CLL /CLR SC
C       3,4, set clock pulse to 0.4096 sec and wait 2 pulses
S     STA;CLZE;CLA CLL;TAD T7;CLDE;JMS CLW;CLA CLL/ SET CLOCK
C       retry just in case it missed 5, set 0420 to zero
C       wait two secs and set 0420 to one
C   !!NOTE BENE!! the digit orders are reversed to allow for wiring
C       error: 0400=E2; 0100=H2; 0040=H1; 0020=K2 all on H808-3
C        and in table 3 in interface manual- table 3( read E2 for F2)
S     TAD MG;DRZ2;JMS CLW;JMS CLW;CLA CLL;TAD MG;DRO2;CLA CLL
C       introduces 90 pulses= 37 second, wait for automatic sample
C       changer- replace by DSCBS signal, which did not work
C       until a diode was put in the line.
      DO 145 J=1,90
S     JMS CLW;CLA CLL
145   CONTINUE
C       reads a/d input from sample changer potentiometer--move earlier
C       lines X=MS;MS=X*A(5)-A(6) to follow here
S     CLA CLL;ADCL;TAD T3;ADLE;ADLM;ADST;A4, ADSK;JMP A4;ADRB;DCA \MS
S     JMP I NXTSA equivalent to fortran RETURN statement
C       constants used in above 7 S lines
S     T2, 6000;T3, 1000;T4, 0400;T5, 0200;T6, 0100;T7, 4400
S     MB, 0100;MR, 0040;MF, 1000;MG, 0420
S     CNTCAL,  0000  /COUNT CALCULATE SUBROUTINE called from SAMCAL
      CALL GKXRSR
      N3=NS(3)
C     XRAY FAULT INDICATION if I returned from GKXSR is 2 or more; sets
C       quartz height to large negative value as indicator of fault
      IF(I-1)131,131,133
133   QH(L9)=-1000-I
C       rings bell for attention to X-ray settings or other fault
      CALL GKXIOP(8)
```

```
C     PEAK NOT DETECTED = NO ANALYTE ie plot doesnt depart significantly
C       from linear in peak range
131   IF(I)130,107,107
130   AR=0
      HT=0
S     JMP I CNTCAL
C     CALCULATE PEAK AREA--normal procedure when result obtained
107   X=0
      Y=0
      W=0
      N1=NS(1)
      N2=NS(2)
      N4=NS(4)
      N5=NS(5)
      DO 109 N=N4,N5
109   X=X+C(N)
      DO 110 N=N1,N2
110   Y=Y+C(N)
      DO 111 N=N2,N4
111   W=W+C(N)
      X1=N5-N4+1
      BL=X/X1/UK
      X1=N2-N1+1
      BR=Y/X1/UK
      X1=N4-N1
      X2=N5-N2
      X3=N4-N2+1
      X4=N5+N4-N2-N1
C       area of peak above background
      AR=W/UK-(BL*X1+BR*X2)*X3/X4
C      background slope
      B1=(BL-BR)/X4*2.
```

```
      X1=N5-N3
      X2=N3-N1
      X3=N5-N1
C       height of peak above sloping linear background
      HT=C(N3)/UK-(BL*X1+BR*X2)/X3
S     JMP I CNTCAL
C       Clock wait subroutine = clock pulse =0.4 second set above
S     CLW, 0000;CLSA;A2, CLSK;JMP A2;JMP I CLW /CLOCK WAIT SR
S     SAMCAL,    0000/ SAMPLE ANALYSIS AND CALCULATION subroutine
C       set first pass count time for weak lines at 8 and strong at 4sec
C       the silver line should be set at KU= 9 to avoid high counts,
C       above 1 000 000, on high accuracy option.
      KU=20
      IF(L2-2)10,11,12
12    IF(L2-5)10,11,13
13    IF(L2-20)10,11,10
11    KU=10
C       sets expected peak angle with correction for undistorted filter
C       displacement below goniometer axis required to avoid damage in
C       insertion into ASC
10    UK=ANG(L2)+A(7)
C       jump to subroutine above
S     JMS CNTCAL
C       check switch register for command abandon-sample-and-rush-to-
C       final-summary table; used when notified of imminent power cut
S     CLA CLL;OSR;AND (2000;SZA;JMP D1;OSR;AND (0400;SZA;JMP TA2
C       set code for output NR NR/100 =line number;middle number is
C       count time code ; peak maximum channel takes value 11 to 19
      L3=LQ(L2)
      J=0
      IF(KU-30)1,1,2
2     J=20
```

```
      IF(KU-120)1,1,3
3     J=40
      IF(KU-480)1,1,4
4     J=60
1     NR(L9)=100*L2+N3+J
C       calcultes weight corresponding to peak area
      X=QM(L2)*FW*1000.
      W=AR*X/A(L3)
      IF(I)164,164,190
C     INTERFERENCE assumed if W less than -.020mg
190   IF(W+20.)191,192,192
191   W=-1000
C       if W between 0 and -.020mg then quartz assumed zero
192   IF(W)193,164,164
193   W=0
C     NORMAL procedure
164   QH(L9)=HT*X/H(L3)
      QS(L9)=W
C     MEAN OF UP TO 4 LINES
C       control for omission on second pass
      IF(J2-2)451,451,454
451   N=L-1
      IF(N)456,456,452
452   DO 453 J=1,N
      Y=QS(L8+J)
C       check for agreement between lines
      X=(W+Y)*.06+20.
      X=ABS(W-Y)-X
      IF(X)118,118,453
C       sum number of lines in agreement and sum weights
118   Q(J2)=Q(J2)+2.
      Q(J2+2)=Q(J2+2)+W+Y
```

```
C       set L5 to control omission of further analyses after agreement--
C       normally goes to minus 1
        L5=L5-1
453     CONTINUE
C       store count data for each quartz line in case agreement not
C       found so that it can be written out and plotted
456     IF(L-4)457,454,454
457     J=L*30+4
        DO 455 N=1,29
455     H(J-N)=C(N)
        H(J)=UK
454     CONTINUE
S       JMP I SAMCAL
C       subroutine DIAG (diagnosis)puts out all data on quartz lines
C        when no agreement is found or when requested
S       DIAG,    0000
C       checks switch register for omit instruction
S       CLA CLL;OSR;AND (0020;SPA CLA;JMP I DIAG
C       outputs 29 counts and other line data and plot for last line
        CALL GKXIOP(4)
C       outputs plots for three preceeding lines
        K1=L-1
        DO 200 K=1,K1
        J=K*30+4
        DO 201 N=1,29
201     C(N)=H(J-N)
        KU=H(J)
        CALL GKXIOP(5)
200     CONTINUE
S       JMP I DIAG
        STOP
        END
```

INPUT OUTPUT SUBROUTINE GKXIO0.

```
C        added comments are in lower case
      SUBROUTINE GKXIOP(J)
C   INPUT OUTPUT PROGRAN FOR X RAY DIFFRACTION GKXMN?-FORTRAN
      COMMON A,AC,NS,C,UK,KU,IR,B,Q,LQ,QM,QS,QH,SD,NR,LS
     C,B1,M,M1,MS,L1,L2,LC,BL,BR,HT,AR
      DIMENSION A(4),AC(24),NS(7),C(29),Q(4),LQ(20),QM(20),QS(12),QH(12)
     C,SD(4,34),NR(12),LS(12),SN(34),KQ(16),KI(4,15)
C       J controls which output routine adopted
      GO TO(51,52,53,54,55,56,57,58,59)J
C       data file contains essential input data see program GKXPD?.FT
C       for description and editing instructions
51    CALL IOPEN('DTAO','GKXIN0')
      READ(4,10)AC,Q,KQ,KI,LQ
C       data file holds useful data on standard intensities for quick
C       reference to check X-ray equipment performance each day
      CALL IOPEN('DTAO','GKXIN1')
      READ(4,9)A,NB
C     SETS CALIBRATION FOR INSTRUMENT AND LINE
510   READ(1,11)I,IR,M1,L1,LS
      READ(1,24)K
      IF(K)510,511,510
511   DO 512 L=1,4
      X=100.
      IF(I)512,512,513
513   X=KI(L,I)
512   QM(L)=Q(L)*X/100.
      DO 514 L=1,L1
      L2=LS(L)
      IF(L2-4)514,514,515
515   L3=LQ(L2)
      X=KQ(L2-4)
```

```
      QM(L2)=QM(L3)*X/50.
514   CONTINUE
C     ENTERS SAMPLE NUMBERS AND WEIGHTS sets default values
      DO 516 K=1,M1
      SN(K)=0
      W=99.99
C       check frontpanel switch register for dont-enter-
C       -sample-numbers-and-weights request
S     CLA CLL;OSR;AND (4000;SZA;JMP TA1;CLA CLL/BYPASSES SAMPLE #S
      WRITE(1,19)K
      READ(1,12)SN(K),W
      IF(W)517,517,516
517   W=.01
C       address for previous S jump instruction
S     TA1,   CLA CLL
516   SD(4,K)=W
C       as above
S     CLA CLL;OSR;AND (4000;SZA;JMP D1;CLA
518   READ(1,24)K,W1,W
      IF(K)519,519,610
610   SN(K)=W1
      IF(W)611,611,612
611   W=.01
612   SD(4,K)=W
      GO TO 518
S     D1,    CLA CLL
519   RETURN
52    RETURN J=2 not used available for extra output routines
53    CONTINUE
C       data output subroutine for reference sample
S     JMS LDATA/   PRINTS STANDARD RESULTS
      WRITE(1,17)A(L2),Q(L2),I
```

```
      RETURN
54    CONTINUE
C       diagnostic print out--when no agreement is found between lines
S     JMS LDATA
S     JMS PLOT
      RETURN
55    CONTINUE
C       another diagnostic printout called from switch register
C       --not used much could be omitted
      WRITE(1,23)M,KU,J,C
S     JMS PLOT
      RETURN
56    CONTINUE
C       normal program output for each sample analysed
S     JMS SAMRES
      RETURN
C       this section produces the normal final table
C       - if the silver line is analysed the absorbtion correction
C       is calaculated using linear regression between sample
C       weight and intensity of the silver line and a second
C       final table is produced with the corrections
57    NB=NB+1
      WRITE(1,15)NB,LC,M
      Y2=2000
      Y0=-2000
S     JMS FINTAB
C       the data from the standard on this batch is stored in file
C       ready for a quick check on the next batch of samples
      CALL OOPEN('DTA0','GKXIN1')
      WRITE(4,9)A,NB
      CALL OCLOSE
S     JMS ABSCOR
```

```
      WRITE(1,18)
S     JMS FINTAB
      RETURN
58    CONTINUE
C       this is intended to attract the technicians attention to
C       an equipment fault -- usually the result of an omitted step
C       in set up
S     CLA CLL;TLS  /RINGS BELL
      DO 580 N=1,50
S     CLA CLL;TAD (0207;JMS TYPE
580   CONTINUE
      WRITE(1,581)
581   FORMAT('XRAY OR INTERFACE FAULT')
      RETURN
59    CONTINUE
      RETURN

C       start of subroutines
S     LDATA, 0000 /DETAILED LINE OUTPUT
C       sample #,line #, I ,29 counts
      WRITE(1,23)M,L2,I,C
C       sample#.count time, 7 peak positions, 2 background slopes,
C       left background, right background, peak height, peak area
150   WRITE(1,19)MS,KU,NS,B,B1,BL,BR,HT,AR
S     JMP I LDATA
C       sample results Normal print-out as each sample is analysed
S     SAMRES,    0000
      DO 551 K=1,2
      X=Q(K)
      Y=-1000
      IF(X)551,551,552
552   Y=Q(K+2)/X
```

```
551   SD(K,M)=Y
C       sample description; net weight; and mean quartz assessment
      WRITE(1,13) SN(M),M,MS,SD(4,M),SD(1,M)
C       code number for line analysed, counting time and peak position
C       QS is sample quartz weight by area and QH that by peak height
C       This output would be improved by using implied DO LOOP to
C       suppress un analysed lines. But didnt function as stated.
      WRITE(1,14)NR,QS,QH
S     JMP I SAMRES

C       Subroutine plots counts versus angle on a printer
S     PLOT,    0000
C       this section determines highest and lowest count
C       and sets zero offset and span for plot.
      X=0
      Y=10.**6
      DO 140 N=1,29
      W=C(N)
      IF(W)140,140,147
147   IF(W-X)141,141,142
142   X=W
141   IF(W-Y)143,140,140
143   Y=W
140   CONTINUE
      IF(X-Y-Y)138,139,139
138   X=Y+Y
139   WRITE(1,25)Y,X
C       this section rejects channels with no count
S     CLA CLL;TLS
      DO 144 N=1,29
      W=C(N)
      IF(W)144,144,148
```

```
148   K=(W-Y)/(X-Y)*70.+1.
C       selects and prints letter for channel number A=1,B=2 etc.
S     CLA CLL;TAD (0300;TAD \N;JMS TYPE
C       prints K blank characters corresponding to count
      DO 146 L=1,K
S     CLA CLL;TAD (0240;JMS TYPE
146   CONTINUE
C       prints asterisk (plot point); carriage return; line feed
S     CLA CLL;TAD (0252;JMS TYPE;TAD (0215;JMS TYPE;TAD (0212;JMS TYPE
144   CONTINUE
S     JMP I PLOT

C       this subroutine prints one character
S     TYPE,    0000;D2,    TSF;JMP D2;TLS;CLA CLL;JMP I TYPE

S     FINTAB,    0000 /summary TABLE AT END OF SAMPLES
      DO 170 K=1,M
      W=SD(4,K)
      X1=SD(1,K)
      X2=SD(2,K)
      Y1=SD(3,K)
C       the next four lines apply the absorbtion correction calculated
C       in subroutine ABSCOR below using Y0 and Y2
      IF(Y0-Y2-Y1)172,172,171
171   Y1=SQRT(Y0/Y1)
      X1=X1*Y1
      X2=X2*Y1
172   X=X1/W/10.
      Y=X2/W/10.
170   WRITE(1,16)K,SN(K),W,X1,X,X2,Y,Y1
S     JMP I FINTAB
```

```
C       This subroutine uses linear regression to correct for absorbtion
C       losses in the dust layer using the intensity of the silver
C       line thru the dust layer
S     ABSCOR,    0000 /ABSORBTION CORRECTION APPROX BEC OF AG TARNISH
      X1=0
      X2=0
      Y1=0
      Y2=0
      DO 180 K=1,M
      Y=SD(3,K)
       IF(Y)181,181,182
181   RETURN
182   W=EXP(SD(4,K))
      X1=X1+W
      X2=X2+W*W
      Y1=Y1+Y
      Y2=Y2+Y*Y
180   XY=XY+W*Y
      X=M
      XY=XY-X1*Y1/X
      X2=X2-X1*X1/X
      Y2=Y2-Y1*Y1/X
      Y0=Y1/X+XY/X2*(1.-X1/X)
      Y2=SQRT((1.-XY*XY/X2/Y2)*Y2/(X-2.))
S     JMP I ABSCOR

9     FORMAT(4A6,A2)
10    FORMAT(28A6,96A2)
11    FORMAT('INSTRUMENT #=',I2.'FILTER TYPE #=',I2/
     C'# OF SAMPLES=',I2,'# OF LINES=',I2.'ORDER OF LINES =',12I2)
12    FORMAT('SAMPLE # A6 &WT F6.2 =',A6,F6.2)
13    FORMAT('S#',A6,2I5,'WT MG=',F7.2,'QZ UG=',F7.0)
```

```
14    FORMAT(I5,11I6,2(/12F6.0))
15    FORMAT('# OF BATCHES =',I6,'LSCF USED',2I5//'SAMPLE #       TOTAL
     CQUARTZ DUST    CRYSTOBALITE    SILVER'/13X,'DUST MG',
     C8X,'UG    %',9X,'UG    %')
16    FORMAT(I2,X,A6,F11.2,2(4X,2F6.0),F10.2)
17    FORMAT('AREA OF STANDARD LAST RUN',F9.1,'MASS',F9.2,I5)
18    FORMAT('ABSORBTION CORRECTED')
19    FORMAT(9I3,2F7.2,4F7.0,/)
24    FORMAT('CONTINUE RTN: AMEND ENT M (S# $ WT)',I2,A6,F6.2)
23    FORMAT(/I3,2I2,9F7.0,2(/10F7.0))
25    FORMAT(/'ANG YAX-XRD XAX MIN=',F7.0,'MX',F7.0/)
      STOP
      END
```

DIFFRACTION LINE ANALYSIS SUBROUTINE GKXSR1.

```
C       new comments are added in lower case and refer to the
C       following section or line
      SUBROUTINE GKXRSR
C     NAME GKXRSR.FT SUBROUTINE FOR COMPUTER CONTROL OF XRAY DIFFRACTION
C       the variables AC and ID are not used in this subroutine
      COMMON AC,NS,C,UK,KU,IR,B,ID
      DIMENSION AC(28),NS(7),C(29),ID(605)
C       OPDEF is operation definition and SKPDF is skip operation
C       definition DRxx is digital input output; xxIx is input;
C       xxZx is zero output by bit for one bit from computer;xxOx is one
C       output by bit for one bit in; xxx? identifies which of three
C       12 bit input outputs is used; CLxx is clock controls
S     OPDEF DRI0 6504;OPDEF DRI1 6514;OPDEF DRI2 6524
S     OPDEF DRZ0 6505;OPDEF DRZ1 6515;OPDEF DRZ2 6525
S     OPDEF DRO0 6506;OPDEF DRO1 6516;OPDEF DRO2 6526
S     OPDEF CLZE 6130;OPDEF CLDE 6132;OPDEF CLSA 6135;SKPDF CLSK 6131
C       default value of probability
      P=2
C       high accuracy option triples counting time( except for the 1,0,1
C       line on the standard); and doubles the probability setting.
C       controlled from front panel switch register but could be
C       requested from the keyboard
S     CLA CLL;OSR;AND (0001;SNA;JMP D5/NORMAL OR HIGH ACCURACY
      KU=KU+KU+KU
      IF(KU-27)81,82,81
82    KU=13
81    P=4
C       wide peak option is useful for distorted filters because of
C       departure from focal plane and for integrating the area
C       over multiple close peaks which cant be resolved.
```

```
C       called from switch register but could be entered from
C       keyboard at start. J3 takes value 4 or 6(option)
S     D5,     ;CLA OSR;AND (0002;IAC;IAC;IAC;IAC;DCA \J3/WIDEN PEAK
C       set variables for start
      DO 100 N=1,29
100   C(N)=0
      I2=0
C       peak centre angle transferred from main
      UANG=UK
      Y=0
C       control for counting time first short then three times
C       longer if required from significance test later
      DO 101 I=1,2
      KU=KU+I2+I2
      I2=I2+KU
      UK=KU
      N2=15-J3
C       Some inconsistency in the use of the numbers 1 to 5 after N
C       starts here. the definitions were given in fig. 5 ref 2
      N3=15+J3                                          N3 to N4
C       count central peak region
      DO 102 N=N2,N3                                    N3 to N4
C       count subroutine
S     JMS ASCT   /COUNTS PEAK
C       sums central region and enters count into array
      Y=Y+W
102   C(N)=C(N)+W
      KU=I2
      UK=KU
      X1=J3+J3+1
      X2=C(N3)+C(N3-1)                                  N4 not N3 twice
      X3=C(N2)+C(N2+1)
```

```
C       sloping linear background
        B=(X2-X3)/(X1+X1-4.)
        Y1=Y/X1
C       mean background
        X2=(X2+X3)/4.
        X1=SQRT(Y1)
C       subroutine finds highest value above sloping linear background
S       JMS MAXVAL /CHECK SIGNIFICANCE OF PEAK
C         divide peak into four regions by curvature
C         1. significantly negative- assume interference. I=1
C         2, insignificant curvature- assume no analyte   I=-1
C         3. recount at longer time -if at maximum time recheck
C            interference or complete processing
C         4. significant complete processing.
C         these choices seem complex but they were introduced
C         to cover the various conditions found.
        IF(Y1-X2+X1)106,103,103
103     IF(X-Y1-8.*X1)104,106,106
104     IF(Y1-X2+P*X1/6.)107,105,105
105     IF(Y1-X2-P*X1)101,106,106
101     CONTINUE
        IF(Y1-X2-0.7*X1)107,107,106
C       IR is used as coded status return signal to the MAIN program
C       -1 is no analyte found
107     IR=-1
        RETURN
C       some confusion over use of N? here see final fig in ref 2
106     IF(N1-3-N2)90,91,91                                  N3 not N1
90      N2=N1-3                                              N3 not N1
91      IF(N1+3-N3)93,93,92                 N3 not N1 and N4 not N3
92      N3=N1+3                             N4 not N3 and N3 not N1
93      CONTINUE
```

```
C       jump to subroutine check interference again
S     JMS INTERF /CHECK INTERFERENCE- FIND SHOULDERS
      NS(6)=N1+8                                              N3 not N1
      NS(7)=N1-8                                              N3 not N1
      NS(1)=N1+3                                              N3 not N1
      NS(2)=N1-3                                              N3 not N1
      DO 150 J=1,7
      X3=NS(1)-NS(2)-1
      B=(C(NS(1))+C(NS(1)-1)-C(NS(2))-C(NS(2)+1))/X3
      DO 151 I=1,2
C       this sets I2 to 1 or -1 to control direction of integration.
      I2=3-I-I
      X2=I2
      IF(NS(5+I)-8*I2-N1)151,152,151                          N3 not N1
152   N=NS(I)
      W=C(N)
      W=W+1.5*SQRT(W)-C(N-I2-I2)-B*X2
      IF(W)153,154,154
153   N=N+I2
C     get count subroutine
S     JMS IFCT
      NS(I)=N
      GO TO 151
154   NS(5+I)=NS(I)-I2-I2
151   N2=NS(6)
150   N3=NS(7)                                                N4 not N3
      X=N2+N2+N2-N3-N3-N3+6                                   N4 not N3 thrice
      B=(C(N2)+C(N2+1)+C(N2+2)-C(N3)-C(N3-1)-C(N3-2))/X       N4 not N3 thrice
C       continues to examine background checking for possible
C       adjacent peaks
S     JMS INTERF /RECHECK INTERFERENCE - BACKGROUND AND PEAKEDGE
      DO 110 I=1,2
```

```
      I2=3-I-I
      J2=(N2-N3)/5+3        N4 not N3
      N=NS(5+I)+I2
S     JMS PKEDGE
      NS(3+I2+I2)=N+I2
      J2=IABS(N-N1)
      IF(J2)135,135,136
135   J2=1
136   I2=-I2
S     JMS PKEDGE
110   NS(3-I2)=N+I2
      B=B/UK
C       normal end of analysis -analyte found in signicant quantity
      IR=0
      RETURN

C       end of main subprogram start of subroutines
C       INTERF checks that peak is within the peak region
C       J3 allows for wide peak option when requested
S     INTERF, 0000;JMS MAXVAL /INTERFERENCE SUB
      N=IABS(N1-15)                                    N3 not N1
C       use IF(J3 -N)continue,return,return
S     CLA CLL;TAD \J3;CIA;TAD \N;SPA CLA;JMP I INTERF
C       interference found return with code IR=1
      IR=1
      NS(1)=N2
      NS(2)=N2+1
      NS(4)=N3-1                                       N4 not N3
      NS(5)=N3                                         N4 not N3
      RETURN

C       finds peak above a sloping background ie searches for
```

```
C       maximum departure above a straight line.
S     MAXVAL,    0000
      X=0
      DO 170 N=N2,N3                                    N4 not N3
S     JMS IFCT
      X3=N-15
      W=W-B*X3
      IF(W-X)170,170,171
171   X=W
      N1=N                                              N3 not N1
170   NS(3)=N1                                          N3 not N1
S     JMP I MAXVAL

C       looks for channel significantly above mean of summed background.
C       the background slope is allowed for.
S     PKEDGE, 0000 /FINDSSTART OF PEAK FOR END OF BKG &SHOULDER
      Y=0
      DO 180 J=1,J2
      X=I2
      N=N+I2
      J1=-2
      IF(N-29)181,182,183
181   IF(N)183,183,182
182   X3=N
S     JMS IFCT
      X1=J
      Y=Y+C(N-I2-I2)-(X3-X-X)*B
      X2=Y/X1+1.5*SQRT(W)
      IF(W-X3*B-X2)180,180,184
184   J1=-3
      IF(C(N-I2)-(X3-X)*B-X2)180,183,183
180   J1=J1+1
```

```
183   N=N+J1*I2
S     JMP I PKEDGE

C       This subroutine checks if channel requested has been counted,
C       If not the count is initated
S      IFCT,    0000  /COUNT IF SUB
      W=C(N)
      IF(W)140,140,141
140   CONTINUE
S     JMS ASCT
141   C(N)=W
S     JMP I IFCT

C       this subroutine converts the angle from binary to BCD on two
C       12 bit outputs; initiates goniometer movement; resets scalar;
C        starts count; times count; stops count; reads count and
C        converts from BCD to binary
S     ASCT,   0000   /ANGLE SET & COUNT SUBROUTINE
C      UANG IS PEAK ANGLE AND AC(8) IS STEP SIZE  .
      DO 133 L=1,5
S     STA;DR00;DR01;CLA CLL  /CLR ANG clears digital output registers;
C     interprets real number angle into two twelve bit binary numbers
C     using integer number truncation to split off decimal fractions
      X1=N-15
      Y1=UANG+AC(8)*X1
      I4=Y1/100.
      X1=I4
      Y1=Y1-100.*X1
      LA=10.*Y1
      X2=LA
      KI=100.*Y1-10.*X2+16.*X1
S     JMS INVER
```

```
      I5=K0
C       this comment gives derivation of split into binary
C       where ABC.DE are five decades each consisting of 4BCD bits
C       except A which is either 0 or 1 ie no angles above 160
C       are possible
C     UANG=ABC.DE: I4=A : LA=BCD :I5=E+16A :I3+I4=256B+16C+D
      I3=LA/100
      I4=LA/10
      I3=96*I3
      I4=LA+6*I4
C     I3 and I4 are used to avoid exceeding 2047, numbers 2048 to 4095
C       are represented internally as negative. KI= the three BCD
C       decades, are set up and maintained on the output register
C       for the PW1394 to read
S     CLA CLL;TAD \I3;TAD \I4;DCA \KI;JMS INVER;CLA CLL /SETS ANGLE &
C        sets up decade E and the 100 output and provides start signal-
C        octal 0002 to H808-2 pin L1 Table 1 in interface manual
S     TAD \K0;DRZ0;CLA CLL;TAD \I5;TAD (0002;DRZ1;JMS CLW;CLA CLL/S SLEW
C        Checks BUSYL signal from PW1394( octal 4000 pin B1 H808-6
C        table 6). this is repeatedfor 20 sec if BUSYL not cleared
C        fault assumed and bell sounded on printer as alarm
      DO 133 K=1,50
S     JMS CLW;CLA CLL;DRI2;AND (4000;SNA;JMP A8 /SLEWED ?
C       codes 2 and higher indicate hardware or system problems
133   IR=3
      RETURN

C     normal procedure continue address when BUSYL cleared
S     A8, CLA CLL
C       try count routines five times-there were lost signal problems
C       may no longer be necessary but why eliminate
      DO 132 L=1,5
```

```
C       clear scalar reset,start and stop signals; operate reset
C       ( octal 2000 H808-3 pinD2 table4) delay 1 clock pulse why?
C       shorter period should clear electronic circuits but not
C       tried. operate start( octal 1000 pin D1)
S     CLA CLL;TAD (7000;DRZ2;JMS CLW;CLA CLL;TAD (2000 /RESET &
S     DRO2;JMS CLW;CLA CLL;TAD (1000;DRO2;CLA CLL /STT COUNTER
      DO 130 K=1,KU
S     JMS CLW;CLA CLL  /0.4 SEC WAIT
130   CONTINUE
C       send stop signal( octal 4000 H808 pinB1). read 3 decades
C       count; convert from BCD to binary  in INVER
S     CLA CLL;TAD (4000;DRO2;CLA CLL;DRIO;DCA \KI;JMS INVER /STP&RD CNT
C       convert to real from binary
      X1=KK
C       next 3 decades D1 is address for a jmp from elsewhere
S     CLA CLL;DRI1;DCA \KI;JMS INVER;D1, 0000;CLA CLL /READS DECS4-6
      Y1=KK
      W=1000.*Y1+X1
C       checks for count if zero- assumed that there was a fault
C       and error message sent to main program IR=4
      IF(W)132,132,131
132   IR=4
       RETURN
C       normal procedure
131   CONTINUE
S     JMP I ASCT

C       clock wait subroutine also checks front panel for interrupt
C       request
S     CLW, 0000;CLSA;A4, CLSK;JMP A4;CLA CLL;OSR;AND (2400;SZA
S     JMP D1;JMP I CLW / CLOCK WAIT SUBroutine clock pulse =0.4096 sec
C       INVER subroutine was written to deal with the wiring error
```

```
C       and the requirement to invert the digit order . It was also
C       found easy to convert the BCD input into binary output at the
C       same time using SABR. KI is input for both. KO is inverted
C       output. KK is inverted and binary output.
S     INVER, 0000;CLA STL RAR;DCA K4  /SR INVERTS DIGIT ORDER KI TO KO &
S     DCA \KO;DCA \KK;IAC;AA, DCA K2  /INVERSE BCD TO BINARY IN KK
S     TAD \KI;AND K4;SNA ;JMP AB   /INPUT DIGIT
S     CLA CLL;TAD K2;TAD \KO;DCA \KO  /OUTPUT DIGIT
S     IAC;DCA K6;TAD K2;AND (0017;SZA;JMP AC /IST DEC
S     TAD (0012;DCA K6;TAD K2;RTR;RTR;AND (0017;SZA;JMP AC /2ND DEC
S     TAD (0144;DCA K6;TAD K2;RTR;RTR;RTR;RTR;   /3RD DEC
S     AC,    CIA;DCA K3;AD,    TAD K6  /MULTIPLY DECADES BY BCD INPUT
S     ISZ K3;JMP AD;TAD  \KK;DCA \KK /BCD OUTPUT IN BINARY
S     AB,    CLL CLA;TAD K4;RAR;DCA K4  /NEXT INPUT DIGIT
S     CLA CLL;TAD K2;RAL;SZA;JMP AA  /NEXT OUTPUT DIGIT
S     CLA CLL;JMP I INVER;
S     K2, 0000;K3, 0000;K4, 0000;K5, 0017;K6, 0000;K7, 0012;K8, 0144
      STOP
      END
```

COMMENTS— There is some confusion in the use of the variable N1 originating in Kemper and van Kempen(3). This was logical in their peak search routine but not in this peak analysis mode . It would be easier to follow if the nomenclature in the last fig in ref. 2 was used, ie N3 and N4 where shown in comments in text.

DATA FILE FOR ANALYSIS GKXIN0.

```
C      printed output requesting create or edit file
FOR NEW DATA FILES ENTER 1;FOR OLD PRESS RETURN
C      printed output giving peak angles for analytes
PEAK ANGLES 2THETA
C    quartz                    : crystobalite          : tridymite
C    1,0,0 1,0,1 1,1,2 2,1,1
#  1 24.24 31.04 58.98 70.96 25.55 33.11 36.69 57.09 27.22 35.22
C    tridymite  :? NaCl and KCl                              ? silver
#  2 45.71 63.71 42.19 55.21 33.05 47.47 59.01 36.93 66.65 44.56
QUARTZ MASSES OF STANDARD
C equivalent determined by calibration with pure quartz samples
#  3  6.19  5.91  7.55  8.72
RATIO OF INTENSITY TO QUARTZ Xs 50
C      times 50 factor used to convert real to integer and save
C      memory on arrays
C      calibration factors for each line
C        5    6    7    8    9   10   11   12  etc
#  4    50  555  416  141  190  286   48  114
#  5   333  117   50  100   25   50   25   50
CALIBRATION RATIOS FOR FOUR LINES ON EACH INST. Xs 100
C      instrument  1       instrument  2       instrument  3 etc.
C      for quartz line with Miller indices -
C      100  101  112  211  100  101  112  211  100  101  112  211

#  6  108  108  108  104  100  100  100  100  100  100  100  100
#  7  114  106  111  112  114  106  111  112  116  108  115  125
#  8  107  108  121  129  131  114  127  133   96   86   96  102
#  9  299  260  291  304  219  196  220  233  112  114  123  133
# 10  100  100  100  100  103  106  106  110  145  145  149  152
AREA OF WHICH QTZ LINE USED IN CALCulation of peak area (and height)
# 11 1 2 3 4 2 2 2 3 2 2 3 4 2 3 2 2 3 2 4 2
REAL CONSTANTS see programs numbers 1,2 are for ASC sample number
C   3 is for filter displacement from axis and 4 is step size angle
# 12  1.00  0.00 -0.30  0.10
ENTER 1 TO15 FOREDIT DATA;16 = END16
```

This data would be more intelligible if prepared as tables and if requested and modified as option from main program. I presume that memory restrictions will be much less and that comments output etc can be made more intelligible.

Suggested tables are 1.
Headings:

line number	; mineral	; Miller index	; peak angle	; calibration line	; ratio to quartz wght	; line intensity
1	quartz	1,0,0	24.24	1	1.0	0
2	,,	1,0,1	31.04	2	1.0	1
3	,,	1,1.2	58.98	3	1.0	0
4	,,	2,1,1	70.96	4	1.0	0
5	crystobalite	?	25.55	2	1.0	1
6	,,	?	33.11	2	11.1	0
7	,,	?	36.69	2	8.32	0
8	,,	?	57.09	3	2.82	0
.....						
13	silver	?	44.56	2	1.0	1

(artificial used only in absorbtion correction)

etc

This table could be more or less unlimited just adding lines as requests for other minerals are received. The ?s can be replaced by looking up the lines in the 'Calculated patterns for silicate minerals'(approx title). The line intensity could be used for setting counting time. Ku=20 for -1; Ku=10 for 0; and KU=9 for 1. The last setting is used to avoid counting over 1 000 000 on very strong lines on the high accuracy option; as required for the 101 line on the reference quartz sample.

The instrument table could have seven headings:- code number; instrument name; version; line 1,0,0; line 1,0,1; line 1,1,2; and line 2,1,1.

The request for table could be y(es) or n(o) and data correction requesting line rewrite line number first. 0 line number means no corrections. See entry correction procedure on data input in GKXIO0.FT

DATA PREPARATION AUXILIARY PROGRAM GKXPD0.

```
C     NAME GKXPD?.FT USED TO PREPARE DATA AND OPEN INPUT FILES
C     FOR XRAY DIFFRACTION GKXMN?.FT
      DIMENSION AC(4),A(10),A1(10),Q(4),KQ(8),KQ1(8),
     CK1(12),K2(12),K3(12),K4(12),K5(12),LQ(20)
      READ (1,9)J
      IF(J)29,29,28
C       file GKXIN1 is only used for performance check data from
C       run to next. It is not maintained through editing
28    CALL OOPEN('DTAO','GKXIN1')
      WRITE(4,10)AC,J
      CALL OCLOSE
      GO TO 30
29    CALL IOPEN('DTAO','GKXINO')
      READ(4,11)AC,A,A1,Q,KQ,KQ1,K1,K2,K3,K4,K5,LQ
      WRITE(1,12)A,A1
      WRITE(1,14)Q
      WRITE(1,16)KQ,KQ1
      WRITE(1,18)K1,K2,K3,K4,K5
      WRITE(1,20)LQ
      WRITE(1,22)AC
30    READ(1,24)I
      GO TO(31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46)I
31    WRITE(1,12)A
      READ(1,13)A
      GO TO 30
32    WRITE(1,12)A1
      READ(1,13)A1
      GO TO 30
33    WRITE(1,14)Q
      READ(1,13)Q
      GO TO 30
34    WRITE(1,16)KQ
      READ(1,17)KQ
      GO TO 30
35     WRITE(1,16)KQ1
      READ(1,17)KQ1
```

```
      GO TO 30
36    WRITE(1,18)K1
      READ(1,17)K1
      GO TO 30
37    WRITE(1,18)K2
      READ(1,17)K2
      GO TO 30
38    WRITE(1,18)K3
      READ(1,17)K3
      GO TO 30
39    WRITE(1,18)K4
      READ(1,17)K4
      GO TO 30
40    WRITE(1,18)K5
      READ(1,17)K5
      GO TO 30
41    WRITE(1,20)LQ
      READ(1,21)LQ
      GO TO 30
42    WRITE(1,22)AC
      READ(1,13)AC
      GO TO 30
43    CONTINUE
44    CONTINUE
45    CONTINUE
46    CALL OOPEN('DTAO','GKXINO')
      WRITE(4,11)AC,A,A1,Q,KQ,KQ1,K1,K2,K3,K4,K5,LQ
      CALL OCLOSE
9     FORMAT('FOR NEW DATA FILES ENTER 1;FOR OLD PRESS RETURN',I2)
10    FORMAT(4A6,A2)
11    FORMAT(28A6,96A2)
12    FORMAT('PEAK ANGLES 2THETA'/'#  1',10F6.2/'#  2',10F6.2)
13    FORMAT('****',10F6.2)
14    FORMAT('QUARTZ MASSES OF STANDARD'/'#  3',4F6.2)
16    FORMAT('RATIO OF INTENSITY TOQUARTZ XS 50'/'#  4',8I5/'#  5'
     C,8I5)
17    FORMAT('****',12I5)
18    FORMAT('CALIBRATION RATIOS FOR FOUR LINES ON EACH INST.'/
     C'#  6',12I5/'#  7',12I5/'#  8',12I5/'#  9',12I5/'# 10',12I5)
```

```
20    FORMAT('AREA OF WHICH QTZ LINE USED IN CALC'/'# 11',20I2)
21    FORMAT('****',20I2)
22    FORMAT('REAL CONSTANTS'/'# 12',4F6.2)
24    FORMAT('ENTER 1 TO15 FOREDIT DATA;16 = END',I2)
      STOP
      END
```

COMMENTS– the explanation of the data edited in this program is given on the print-out of the DATA file GKXRIN0.DA together with suggested changes given on pages 31 to 32.

```
20    FORMAT('AREA OF WHICH QTZ LINE USED IN CALC'/'# 11',20I2)
21    FORMAT('****',20I2)
22    FORMAT('REAL CONSTANTS'/'# 12',4F8.2)
24    FORMAT('ENTER 1 TO15 FOREDIT DATA;16 = END',I2)
      STOP
      END
```

COMMENTS

The explanation of the data edited in this program is given on the printout of the DATA file GKXRINO.DA together with suggested changes given on pages 31 to 32.

APPENDIX XRD VARIABLES –

correlation between subroutines – in COMMON statement

GKXMN	GKXIO	GKXSR	GKXPD	GKXPD	Description of variables
			file0	file1	data files on tape created by GKXPD?.FT
A(4)	A(4)	AC(28	A(4)		storage of peak areas between runs
A(5-8)	AC(4)	not		AC(4)	input– constants - step size etc.
ANG(20)	AC(5-24)	used)		A(10)	input– peak angles for the 20 lines analysable
				A1(10)	
NS(7)	NS(7)	NS(7)			channel numbers describing peak shape
C(29)	C(29)	C(29)			count in each channel
UK	UK	UK			counting time –real /transfer angle MN to SR
KU	KU	KU			counting time – integer = clock pulses =0.4096sec
I	IR	IR			status code number
B	B	B			Background height – average
Q(4)	Q(4)	ID(605		Q(4)	input–equivalent mass of standard on four lines
					output–averaging of lines in agreement
LQ(20)	LQ(20)			LQ(20)	which of the four quartz lines to be used as standard
QM(20)	QM(20)				input–equivalent mass of standard for analyte and line
QS(12)	QS(12)				output–mass of analyte from area under peak
QH(12)	QH(12)				output–mass of analyte from peak height
SD(4,34)	SD(4,34)				storage of counts and line data for quartz– used when interference found ie no agreement
NR(12)	NR(12)				output–code giving line number (times 100) code for counting time (x1x lowest x3x next etc) and peak channel no(11 to 19)
LS(12)	LS(12)	not			input– order of lines for analysis
B1	B1				slope of background under peak
M	M				sample no of sample being analysed –standard = 0
M1	M1				input –number of samples in batch
MS	MS				sample no read from auto. samp. changer– not operative slip on potentiometer drive -uses 2 constants in AC
L1	L1				input– number of lines to be analysed
L2	L2				active line
LC	LC				output– use of light sample correction factor
BL	BL				background on left(low angle) side of peak
BR	BR				ditto on right
HT	HT				height of peak above background
AR	AR	used)			integrated area of peak above background

correlation between subroutines – direct

GKXMNGKXIO	GKXSRGKXPDGKXPD	Description of variables
	file0 file1	data files on tape created by GKXPD?.FT
NB	J	batch no– program generated
KQ(8)	KQ(8)	coded factor for equivalent quartz mass for each line
KQ(9-16)	KQ1(8)	– = factor times 50
KI(4,15)	K1(12)	coded instrument calibration factors
	TO	– 15 samplers 4 lines each
KI	K5(12)	– = factor times 100
call no J		output– controls which print out routine used

GKXMN?.FT Description of Variables in MAIN Program

variable	description
L	used as line variable sometimes
L1	input– number of lines to be run
L2	active line for standard and sample
L3	specific quartz line used in determination of analyte mass = LQ(L2)
L5	controls diagnostic print out from panel switch(0300)and program response to interference – no agreement between 4 lines
L7	control to stop running line in smaller group of 4 than appropriate
L8	line control for groups of 4. required when less than 4 lines called for in group
L9	line number used in DO 404 loop
LC	output– indicates use of light sample correction factor in results
SD(1,M)	mean quartz weight for sample M
SD(2,M)	mean crystobalite weight
SD(3,M)	relative intensity of silver peak measured thru dust layer for absorbtion correction
SD(4,M)	net gravimetric weight of sample
Q(1)	no of lines in agreement contributing to mean quartz
Q(2)	sum of quartz weights in agreement– mean = Q(1)/Q(2)
Q(3)	as Q(1) for crystobalite
Q(4)	as Q(2) for crystobalite
N1	=NS(1) channel number at low angle edge of integrated background
N2	=NS(2) ditto low angle edge(shoulder) of integrated peak
N3	=NS(3) ditto maximum peak height
N4	=NS(4) ditto high angle edge of peak
N5	=NS(5) ditto high angle edge of integrated background